

A Review of the Kinetic Statistical Strength Model

Armand V. Attia

March 11, 1996



This is an informal report intended primarily for internal or limited external distribution. The opinions and conclusions stated are those of the author and may or may not be those of the Laboratory.

This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This report has been reproduced
directly from the best available copy.

Available to DOE and DOE contractors from the
Office of Scientific and Technical Information
P.O. Box 62, Oak Ridge, TN 37831
Prices available from (615) 576-8401, FTS 626-8401

Available to the public from the
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Rd.,
Springfield, VA 22161

A REVIEW OF THE KINETIC STATISTICAL STRENGTH MODEL

Armand V. Attia

Introduction.

This is a review of the Kinetic-Statistical Strength (KSS) model, described in the report: "Models of Material Strength, Fracture and Failure" by V. Kuropatenko and V. Bychenkov¹. The report covers several approaches to material strength modeling for simulating the dynamic response of metals to explosive charges and the rock response to underground explosions. I have focussed on the material strength models for metals subjected to high strain rates, leaving an evaluation of rock response for later review.

This review traces the theoretical development of the KSS model, which has been validated against two types of experiments on metal response to shock loading: (1) rupture time vs. tensile stress, and (2) spatial attenuation of elastic precursor peak stress.

Model Overview.

The original KSS model described by Zhurkov² was found to apply only to quasi-static loading. Improvements were made by Sanin³ to extend the model to dynamic loading. Gornovoi⁴ modified the model to describe the attenuation of the elastic precursor in the response of metals to explosive charges. Finally, Kuropatenko and Bychenkov¹ show how to incorporate the model into an elasto-plastic stress advance formulation.

Quasi-Static Model

In Zhurkov's model, material strength is characterized by *durability* τ . This is the time for a material sample to fail, when it is subjected to a rectangular tensile *pulse* sufficiently high to reach the material ultimate strength σ . During a *static* tensile test, ultimate strength is the maximum load divided by original sample cross-sectional area. The quasi-static KSS model is based on an *empirical* relationship² between the durability τ and the tensile ultimate strength σ :

$$\tau = \tau_0 \exp (U_0 - \gamma\sigma)/kT \quad (1)$$

where τ_0 is the period of thermal oscillation of atoms in a crystal lattice, U_0 is the energy of interatomic bonds, γ is the activation volume (see below), k is Boltzmann's constant, and T is the temperature.

Zhurkov⁵ interprets U_0 as ϵ^*c_a/α and γ as $(c_a/\alpha E)\kappa$, where ϵ^* is the breaking strain of an atomic bond, c_a is the atomic specific heat, α is the coefficient of thermal expansion, E is the elastic Young's modulus, and κ is a "mechanical overload factor".

Later, Zhurkov² identifies this factor κ as Λ/a , the ratio of a *phonon*⁸ *mean free path* Λ to the atomic radius a . It is here that Zhurkov refers to the notion of a *dilaton*. This notion was discussed in earlier work by Kusov⁷, who describes the breaking of a loaded chain of vibrating atoms, as a result of thermally-induced negative fluctuation in the atomic density.

A *dilaton* is a strained region of the atomic lattice. The straining is assumed to result from density fluctuations caused by spontaneously random atomic motion, or equivalently as a result of the superposition of elastic waves describing lattice vibrations. The volume v_d of a dilaton is a cylinder of height Λ and cross-section a^2 . Thus, the dilaton is the minimum volume over which phonons can collide. The dilaton can be an incubator for crack nucleation. The strained region may develop into a phonon trap, allowing phonon energy to accumulate until this energy reaches the critical value for a crack to nucleate. Before the crack nucleates, interatomic bonds are stretched for duration τ by an amount $\epsilon_d = (\alpha T/3)\ln(\tau/\tau_0)$. The dilaton tends to be short lived with decay lifetime $\tau_d = \Lambda/c$ of the order of 0.1 to 1 ns, where c is the sound speed in the material.

Finally, Zhurkov² also shows that for long durabilities (1 sec.), the quasi-static model agrees well with experimental data (see Fig. 1), for the temperature dependence of breaking strength for aluminum, copper, nickel, steel, and molybdenum.

Extension to Dynamic Model

Sanin³ recognized that Zhurkov's model applied mainly to long durabilities, down to about 1 ms. For shock loading, the model needed to be extended to durabilities below 1 microsec.

Several notions were involved in making this extension. The starting point was the quasi-static model with the notion of a dilaton as an incubator for crack nucleation, as discussed above. Two developments were required: (1) how to apply the KSS model to actual material sample size, obviously several orders of magnitude bigger than the tiny dilaton, and (2) how to apply *static* strength data to *shock* response. Finally, these notions were incorporated within Zhurkov's KSS framework to complete the dynamic model.

Scale effect

For the first requirement, Sanin uses Weibull's statistical model⁶ for relating strength to material sample volume. According to Weibull (see also Timoshenko⁹), since the strength of brittle materials is influenced by the presence of imperfections, we can expect that the ultimate strength will depend on the size of the specimen, so that the material tends to be weaker, as the specimen gets larger, since the probability of defects then increases. Weibull developed a statistical model, for *brittle* materials, relating ultimate strength σ to sample volume v , so that for two samples 1 and 2:

$$\sigma_1/\sigma_2 = (v_2/v_1)^{1/\alpha_u} \quad (2)$$

where α_u is determined by relating stress vs. volume at the atomic and actual sample scales. For this purpose, Sanin first rewrites (1) in the form:

$$\sigma = \frac{\epsilon^* E}{\kappa} \left(1 - \frac{\alpha k T}{\epsilon^* c_a} \ln \frac{\tau}{\tau_0} \right) \quad (3)$$

Consider a material specimen with volume v_0 . Recall that $\kappa = \Lambda/a$, where the phonon mean free path Λ can also be viewed as an indication of structural non-uniformities in the body for the volume v_0 . Thus, κ is a function of the specimen volume; i.e. $\kappa = \kappa(v_0)$. Sanin now uses the definition that the dilaton has the smallest volume over which phonons may interact. This dilaton volume v_d is

related to the atomic volume with the same scale of non-uniformities as for the entire specimen volume. In fact, $v_d = \Lambda a^2 = (\Lambda/a)a^3$ so that:

$$v_d = \kappa(v_0)v_a \quad (4)$$

Thus, if we now consider a tiny material sample of volume v_d , we must then have:

$$\kappa(v_d) = 1, \quad (5)$$

and the local dilaton stress σ_d is obtained from (3) using (5). Now, given a material specimen of volume v_0 and ultimate strength σ_b , the Weibull model relates the dilaton sample to the actual sample by:

$$\sigma_b/\sigma_d = (v_d/v_0)^{1/\alpha_u} \quad (6)$$

Using (4) in (6) and rearranging gives:

$$(\sigma_d/\sigma_b)^{\alpha_u} = (v_0/v_a)/\kappa(v_0) \quad (7)$$

But, from the inverse relation between σ and κ in (3):

$$\kappa(v_d)/\kappa(v_0) = \sigma_b/\sigma_d \quad (8)$$

Now, using (5) in (8), solving for $\kappa(v_0)$, and putting this result into (7) gives the required expression for α_u as:

$$\alpha_u = \frac{\ln(v_0/v_a)}{\ln(\sigma_d/\sigma_b)} - 1 \quad (9)$$

Having determined α_u from some subset of specimens, we then expect that the Weibull model will correctly predict the strength of remaining specimens.

Shock response

Sanin addresses the second requirement, for how to apply static strength data to shock response, by noticing an important contrast between static and shock loading. In *static loading*, the first microcrack occurs at the site with greatest number of defects in the site volume. Under static test conditions, the defect grows into a Griffith crack, which (at some critical size) will propagate with

velocity of about 0.4 c. Thus, for a static test, the appropriate volume of material to consider is the entire volume of the body under load.

In order, to describe *impulsive loading* under statically equivalent conditions, Sanin assigns the cylindrical volume of radius $c\tau$ and height $0.4c\tau$ to the volume v (approximately $0.5 c^3\tau^3$) of that part of the body under impulsive load. Now subdivide the loaded part of the body into N elementary volumes v such that during the time τ , they don't interact. The strength of the individual elements of such a statistical ensemble will be determined by the population of defects in each element. In shock loading, as the shock sweeps across the material, the process of fracture within individual volumes will be associated with multiple sites. Thus, shock loading leads to multiple sites for crack nucleation, while static loading leads to a single nucleation site.

Now, from (5) and the inverse relation between σ and κ in (3), we have:

$$\kappa(v) = (v/v_d)^{1/\alpha_u} \quad (10)$$

or, with the cylindrical volume of $v=0.5 c^3\tau^3$, we have:

$$\kappa = (0.5 c^3\tau^3/v_d)^{1/\alpha_u} \quad (11)$$

Putting (11) into (3) gives:

$$\sigma = E \varepsilon^* (2v_d/c^3\tau^3)^{1/\alpha_u} \left(1 - \frac{\alpha k T}{\varepsilon^* c_a} \ln \frac{\tau}{\tau_0}\right) \quad (12)$$

which is valid while these cylindrical volumes v do not interact; i.e., while

$$0.5 c^3\tau^3 < v_0 \quad (13)$$

where v_0 is the volume of material subjected to shock loading. Now, when $0.5 c^3\tau^3 = v_d$, we have $\kappa(v) = 1$, and (12) determines the decay of the local dilaton stress σ_d . Then, later, when $0.5 c^3\tau^3 = v_0 \gg v_d$, Equ. (12) becomes Zhurkov's quasi-static equation (1) with:

$$U_0 = \varepsilon^* c_a / \alpha \quad (14a)$$

$$\gamma = (c_a / \alpha E) (v_0 / v_d)^{1/\alpha_u} \quad (14b)$$

Note that (14a-b) correspond to Zhurkov's interpretation, above. However, Sanin has now incorporated into Zhurkov's framework the notions of scale and time, allowing the model to be considered for actual material samples subjected to either shock loading or quasi-static loading, where there is now a threshold durability τ^* , with the following role. For $\tau < \tau^*$, we need the explicit time dependence for the pertinent growing volume v and associated overload factor $\kappa(v)$. For $\tau > \tau^*$, we want a constant value for that volume, associated now with the entire specimen, since by that time all elemental cylindrical volumes have communicated. This notion becomes important in applying the KSS model to elasto-plastic stress advance, as described below.

Sanin compares the extended model favorably with experimental data (see Fig. 2) for dependence of durability vs. cleavage resistance of copper, steel, and an alloy (V95).

Attenuation of Elastic Precursor

Before describing the application of the KSS model to elasto-plastic response, let's take a look at a new vantage point that the KSS model provides on the roles of elastic and plastic behaviors. Gornovoi⁴ adapted the dynamic model to describe the attenuation of the elastic precursor in the response of metals to explosive charges, using:

$$\sigma_{xx}^e = E \frac{1-\nu}{1-2\nu} (v_d/c^3 \tau^3)^{1/\alpha_u} (\varepsilon^* - \frac{\alpha k T}{c_a} \ln(\tau/\tau_0)) \quad (15)$$

where σ_{xx}^e is the amplitude of the Hugoniot elastic limit, ν is Poisson's ratio, E is Young's modulus, v_d is the dilaton volume, c is the longitudinal elastic wave speed, and where τ is now the time for the local lattice strain to reach the critical value ε^* . Gornovoi thus describes the effect of this local plastic deformation on the Hugoniot elastic limit. The formation of a plastic region can be seen as starting with the accumulation of elastic energy into a dilaton (i.e. phonon pumping) and finally releasing this accumulated energy when bonds are broken.

Gornovoi compares this model with experimental data (see Fig. 3), obtaining good agreement for the spatial attenuation of elastic precursor stress in metal wedges subjected to explosive charges, for steel, titanium BT1-00, and its alloy BT3-1.

Elasto-Plastic Stress Advance

The incorporation of the KSS model into an algorithm for the SPRUT code to describe the elasto-plastic advance of stress deviators is developed by further modifying the theoretical formulation. In summary, Sanin's KSS model is "generalized" (see Eq. (3.9) in Reference 1), and a KSS-based flow rule (see Eq. (3.15) in Reference 1) is obtained, within the context of Prantl-Reiss relations, where the yield surface is allowed to change with time. Then, the "generalized" KSS model is rewritten into a "relaxation" form (see Eq. (7.1) in Reference 1), in which breaking strain ε^* is replaced with a corresponding form using the dynamic yield strength Y . Finally, the "relaxation" form is implemented in the SPRUT code (see Section 5.2, Step 7.3, in Reference 1).

"Generalized" model

The generalized KSS model takes the form:

$$\ln (\tau/\tau_0) = (T^*/T_0) (\varepsilon^* - k(\sigma/M) (\tau/\tau_0)^\beta) \quad \text{for } \tau \leq \tau^* \quad (16a)$$

$$\ln (\tau/\tau_0) = (T^*/T_0) (\varepsilon^* - k(\sigma/M) (\tau^*/\tau_0)^\beta) \quad \text{for } \tau > \tau^* \quad (16b)$$

The coefficient $k = (c_1 \tau_0 / v_a^{1/3})^\beta$, c_1 is the longitudinal sound speed, and $\beta = 3/\alpha_u$. The temperature $T^* = c_p/\alpha R$; T_0 is not defined, but it is probably the temperature associated with the quasi-static (isothermal) measurements of the strength σ . A non-linear relation is obtained for the durability τ^* across the static/dynamic regimes, so that given tensile strength σ_0 and yield strength Y_0 , from static tests, τ^* is given respectively by :

$$\ln (\tau^*/\tau_0) = (T^*/T_0) (\varepsilon^* - k(\sigma_0/M_{01}) (\tau^*/\tau_0)^\beta) \quad (17a)$$

$$\ln (\tau^*/\tau_0) = (T^*/T_0) (\varepsilon^* - k(Y_0/M_{02}) (\tau^*/\tau_0)^\beta) \quad (17b)$$

where the associated moduli are given by $M_{01} = K + (4/3)\mu$ and $M_{02} = 2\mu$, K is the bulk modulus, and μ is the shear modulus.

In order to obtain a flow rule, from this "generalized" KSS model, a non-linear relaxation relation between stress and durability is

derived by differentiating (16a) or (16b), for fixed temperature T , critical strain $\epsilon=\epsilon^*$, and modulus M , giving:

$$d\sigma/d\tau = -\beta^* \sigma/\tau \quad (18)$$

where σ is peak tensile strength, in the case of tensile failure, and σ is proportional to the second invariant of stress deviators, for shear failure, and where β^* is determined by:

$$\beta^* = \beta + \frac{1}{(\epsilon T^*/T - \ln(\tau/\tau_0))} \quad \text{for } \tau \leq \tau^* \quad (19a)$$

$$\beta^* = \frac{1}{(\epsilon T^*/T - \ln(\tau/\tau_0))} \quad \text{for } \tau > \tau^* \quad (19b)$$

A flow rule, similar to the Prandtl-Reiss relation, is now obtained in the form:

$$dS_{ij}/dt = 2\mu e_{ij} - (\beta^*/\tau)S_{ij} + \omega_{ik} S_{kj} + \omega_{jk} S_{ki} \quad (20)$$

where e_{ij} is the deviatoric strain rate, S_{ij} is the deviatoric stress, ω_{ij} is the anti-symmetric part of the velocity gradient, and μ is the shear modulus.

"Relaxed" model

The "generalized" KSS model (16a-b) is rewritten into a "relaxation" form, in which breaking strain ϵ^* is replaced with a corresponding form using the dynamic yield strength Y , giving:

$$2\mu(T/T^{**}) \ln(\tau/\tau_0) = Y (\tau^*/\tau_0)^\beta - J (\tau'/\tau_0)^\beta \quad (21)$$

where $\tau' = \tau$ if $\tau \leq \tau^*$, and $\tau' = \tau^*$ if $\tau > \tau^*$, and where $T^{**} = (c_p/\alpha R)(c_1 t_0/v_a^{1/3})^\beta$, t_0 is the current problem time, c_1 is the sound speed, $J = (1.5 S_{ij} S_{ij})^{1/2}$, and S_{ij} are the stress deviators. The intent of this model is to prescribe the tendency of the stress deviators to relax toward a dynamic yield limit, which is defined only when $\tau > \tau^*$. Then, the *dynamic* yield limit is calculated by solving (21) for Y , where J is now the *measured quasi-static* yield

limit. Otherwise, if $\tau \leq \tau^*$, there is no constraint on the elastically advanced stress deviators.

SPRUT implementation

Given J^{n+1} for the *elastically* advanced stress deviator S_{ij}^{n+1} , and (assuming that $Y = Y^n$), Equ. (21) is solved iteratively for the relaxation time τ^{n+1} . A new yield limit Y^{n+1} is then determined to be $J(\tau^{n+1} + \Delta t_0)$, using (21) with $Y = Y^n$, where Δt_0 is a fraction of the current time step. If $Y^{n+1} > J^{n+1}$, no deviator adjustment is necessary. Otherwise,

$$\Delta S_{ij} = S_{ij}^{n+1} (Y^{n+1}/J^{n+1} - 1) \quad (22)$$

Conclusion

This completes a review of the Kinetic Statistical Strength model. Model implementation appears to be possible in a hydrocode. Applying the model to the shock response of metals will require a data source for the Weibull parameter α_u , short of measuring the strength of specimens of various sizes. Model validation will require more details on the experiments successfully calculated by SPRUT. Beyond validation, we need to evaluate the KSS model against other existing rate-dependent models for metals such as the Steinberg-Lund model¹⁰, or the MTS¹¹ model, on other shock experiments.

References.

(Russian citations apply to English translations, except as noted)

1. V. Kuropatenko, V. Bychenkov, "Models of Material Strength, Fracture, and Failure", Report under contract B239597, item 01, Russian Federal Nuclear Centre, All-Russian Institute of Technical Physics, 23 May 1995.
2. S. N. Zhurkov, "Dilaton mechanism of the strength of solids", *Sov. Phys. Solid State*, Vol. 25, n. 10, p. 1797, 1983.
3. I. V. Sanin, A. I. Vorob'ev, A. A. Gornovoi, "Kinetic-statistical model of the cleavage of metals", *Sov. Combustion, Explosions, and Shock Waves*, Vol. 23, n. 1, p 61, 1986.

4. A. A. Gornovoi, E. A. Kozlov, A. K. Muzyrya, E. V. Shorokhov, "Investigation of the relaxation kinetics of an elastic predecessor in Steel 3 and Titanium", *Sov. Combustion, Explosions, and Shock Waves*, Vol. 25, n. 1, p. 131, 1989.
5. S. N. Zhurkov, "Physical basis of the strength of materials", *Sov. Phys. Solid State*, Vol. 22, n. 11, p. 1958, 1980.
6. V. V. Bolotin, Statistical methods in structural mechanics, Holden-Day, 1969.
7. A. A. Kusov, "Phonon model of breaking of a loaded atomic chain", *Sov. Phys. Solid State*, Vol. 21, n. 10, p. 1781, 1979.
8. C. Kittel, Introduction to Solid State Physics, Wiley, 1986.
9. S. Timoshenko, Strength of Materials, Part II, Van Nostrand, 3rd edition, 1958.
10. D. J. Steinberg, C. M. Lund, "A constitutive model for strain rates from 10^{-4} to 10^6 s $^{-1}$ ", *J. Appl. Phys.*, Vol. 65, n. 4, p. 1528, 1989.
11. P. S. Follansbee, U. F. Kocks, "A constitutive description of the deformation of copper based on the use of the mechanical threshold stress as an internal state variable", *Acta metallica*, Vol. 36, n. 1, p.81, 1988.
12. V. I. Romanchenko, G. V. Stepanov, "Dependence of the critical stresses on the loading time parameters during spall in copper, aluminum, and steel", *J. Appl. Mechanics and Technical Physics*, n. 4, p. 555, July-Aug. 1980.
13. A. G. Ivanov, S. A. Novikov, V. A. Sinitsyn, "Elastoplastic waves in iron and steel during explosive loading", *Fizika Tverdogo Tela*, Vol. 5, n. 1, p. 269, 1963. [Original Russian publication].

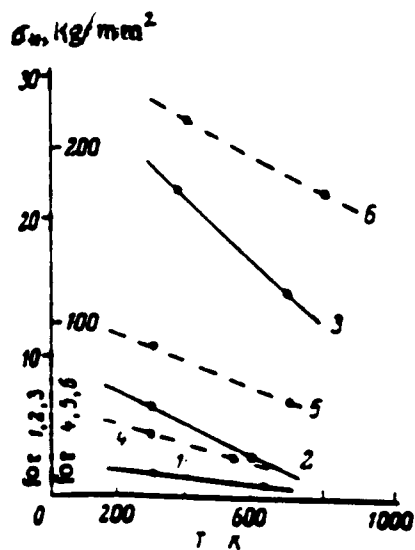


Fig. 1. Temperature dependences of breaking strength². Calculations are shown as points on lines of observations. Solid lines : (1) sodium chloride, (2) aluminum, (3) copper. Dashed lines: (4) nickel, (5) steel-3, (6) molybdenum.

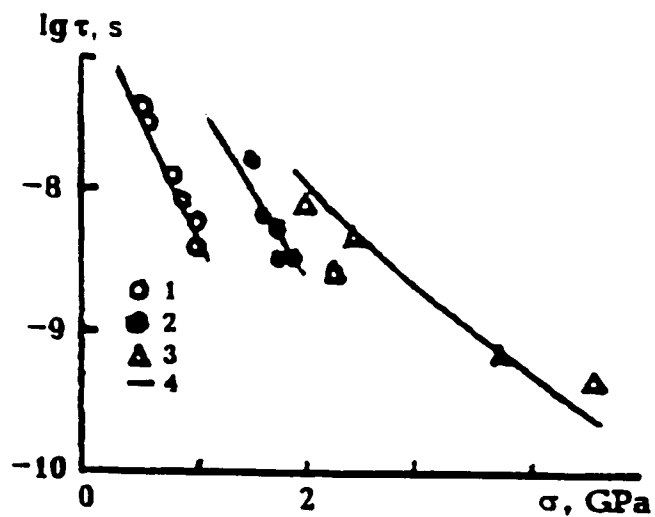


Fig. 2. Dependence of critical stresses on the time parameter of load at failure.³ Calculations³ are shown as lines. Observations¹² are shown for: (1) copper, (2) alloy V95, (3) steel.

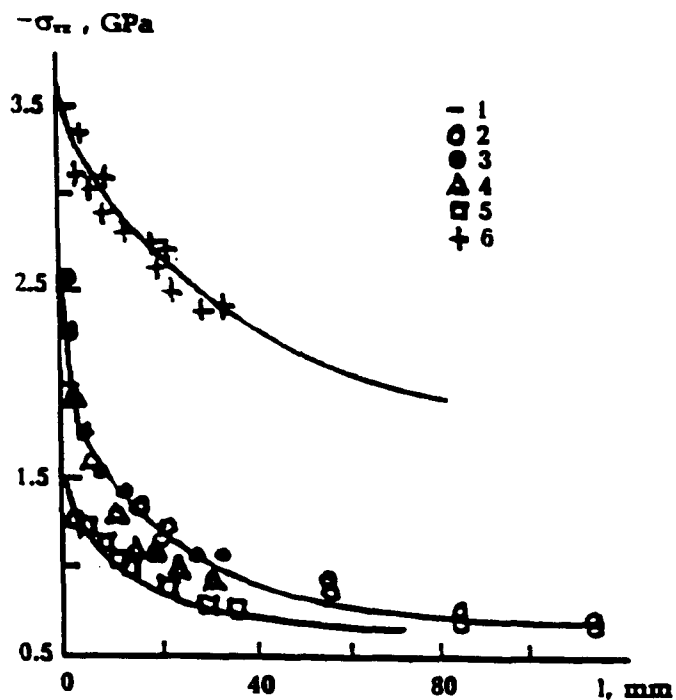


Fig. 3. Attenuation of elastic precursor⁴.
 Calculations⁴ are shown as lines (1).
 Observations are shown for various impulsive loads P_0 :
 (2) steel¹³ 3 with $P_0 > 15$ GPa;
 (3) steel⁴ 3 with $P_0 > 15$ GPa;
 (4) steel⁴ 3 with $P_0 < 10$ GPa;
 (5) titanium VT1-00¹³ with $P_0 < 10$ GPa;
 (6) titanium alloy VT3-0¹³ with $P_0 < 10$ GPa;